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UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY (EPA)
HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For The

HIGHER OLEFINS CATEGORY

Prepared by:

American Chemistry Council
Higher Olefins Panel

July **5, 2001**

EXECUTIVE SUMMARY

The Higher Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the test plan for the Higher Olefins category under the United States Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analyses to adequately characterize the OECD SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category.

This test plan addresses alpha and internal aliphatic olefins, linear and branched, which are within the HPV Challenge Program. The members of the category fall within the ranges of even carbon numbers for C6 – C54 alpha olefms, C 13 alpha olefins, and C6 – Cl 8 internal olefins (odd and even carbon numbers). The C6 – Cl4 even numbered linear alpha olefins are sponsored under the SIDS program. The Panel has committed to sponsor the C6, C7, C8, C9, and Cl2 aliphatic linear and branched internal olefins and the Cl 6 and Cl 8 aliphatic linear alpha olefins in the ICCA HPV program.

The test plan is based on the expectation that internalizing the location of the carbon-carbon double bond, increasing the length of the carbon chain, and/or changing the carbon skeleton's structure from linear to branched does not change the toxicity profile, or changes the profile in a consistent pattern from lower to higher carbon numbers.

This plan addresses identified testing needs of the category by filling relevant data gaps at the upper and lower ends of the homologous series of Higher Olefins. At the lower end of the homologous series, three tests will be conducted with a C6 internal olefin stream (approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes, 60-74% branched) to include invertebrate acute toxicity, alga toxicity, and 28-day repeated dose rat oral/neuro/reproduction/developmental toxicity screen (OECD 422). For the upper end of the homologous series, a rat oral reproduction/developmental toxicity screen (OECD 42 1) will be conducted with a Cl8 internal olefin (20-30% branched). The results of these tests will be compared with available data for other homologs within the series of olefins. If the results from the above testing confirm that the toxicity profiles of all members of the Higher Olefins category are essentially the same, or a pattern from lower to higher carbon numbers exists, any remaining data gaps can be considered to fall within the ranges defined by the data and no further testing will be warranted. If the results do not confirm that hypothesis, a reassessment of the category will be conducted.

Predictive computer models will be used to develop relevant environmental fate and physicochemical data for chemicals in the Higher Olefins category. Environmental fate information will be summarized either through the use of computer models when meaningful projections can be developed or in technical discussions when computer modeling is not applicable. For mixed streams, physicochemical properties will be represented as a range of values according to component composition. These data will be calculated using a computer

model cited in an EPA guidance document prepared for the HPV Challenge Program. In addition, measured physicochemical data will be provided for selected product streams in this category where readily available.

American Chemistry Council's

HIGHER OLEFINS PANEL

The Higher Olefins Panel includes the following member companies:

BP

Chevron Phillips Chemical Company LP

CONDEA Vista Company

ExxonMobil Chemical Company

Shell Chemical Company

Shell Chemicals Ltd.

Sasol

Spolana a.s. Neratovice

Sunoco, Inc.

TABLE OF CONTENTS

TEST PLAN FOR THE HIGHER OLEFINS CATEGORY

TEST PLAN FOR THE HIGHER OLEFINS CATEGORY

I. INTRODUCTION

The Higher Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical test data for the Higher Olefins category under the United States Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program (Program).

This plan identifies CAS numbers used to describe substances in the category, identifies existing data of adequate quality for substances included in the category, and outlines testing needed to develop screening level data for this category under the Program. This document also provides the testing rationale for the Higher Olefins category. The objective of this effort is to identify and develop sufficient test data and/or other information to adequately characterize the human health and environmental effects and fate for the category in compliance with the EPA HPV Program. Physicochemical data that are requested in this program will be calculated as described in EPA guidance documents. In addition, measured physicochemical data will be provided for selected product streams in this category where readily available.

II. BACKGROUND

Most higher alpha olefins are manufactured on a commercial scale by oligomerization of ethylene or propylene. The materials produced are mixtures including a range of molecular weights. These broad mixtures can be subsequently distilled into narrower mixtures or discrete chemical substances. The internal olefins are made from alpha olefins by isomerization or by isomerization/disproportionation, which can result in mixed chain length internal olefins. Oligomerization of ethylene generally leads to linear alpha olefins. Certain branched structures are also produced, typically as minor components, though levels increase with molecular weight and can be significant. Oligomerization of propylene generally produces branched alpha olefins. Various degrees of alkyl chain branching can be introduced by catalytic isomerization of linear oletins.

Two other routes to higher olefins are of commercial significance. Mixed alpha olefins are produced from synthesis gas (carbon monoxide and hydrogen) via Fischer-Tropsch type oligomerization. Internal olefins are produced from normal paraffins by partial catalytic dehydrogenation. Commercially valuable components are obtained via distillation or molecular sieve extraction followed by one or more purification steps.

Commercial higher olefins thus can range from narrowly defined substances to complex mixtures of alpha and internal, linear and branched oletins characterized by carbon range and physical properties.

III. DESCRIPTION OF THE HIGHER OLEFINS CATEGORY

This test plan addresses aliphatic alpha and internal olefins, linear and branched, which are within the HPV Challenge Program. The members of the category fall within the ranges of C6 – C54 alpha olefins (even carbon numbers except for C 13) and C6 – Cl8 internal olefins (odd and even carbon numbers). The C 16, Cl 8, and C20-24 alpha olefins are linear. Neohexene is branched. The C24 – C54 alpha olefins fraction is a mixture of branched and linear isomers. The internal olefins are mostly linear, mostly branched, or a mixture of linear and branched isomers. The members of the category are presented in Table 1.

Table 1: Members of the Category

Alpha Olefms	**Branched/Linear**	CAS No.
Neohexene	Branched	558-37-2
1 -Tridecene	Linear	2437-56-1
1 -Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-g
1 -Eicosene	Linear	3452-07-1
1 -Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
Internal Olefins		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	Branched and Linear	68526-53-4
Alkenes, C7-9, C8-rich	Branched and Linear	68526-54-5
Alkenes. C8-10. C9-rich	Branched and Linear	68526-55-6
Alkenes, C9- 11, C 1 O-rich	Branched and Linear	68526-56-7
Alkenes, C 10- 12, C 11 -rich	Branched and Linear	68526-57-8
Alkenes, C 1 1 - 13, C 12-rich	Branched and Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-l O-8
Alkenes. C 10- 16	Linear	6899 l-52-6
Alkenes, C 15-C 18	Linear	93762-80-2
C 10,12 Olefin rich hydrocarbons	Linear	685 14-32-9
C 12,14 Olefin rich hydrocarbons	Linear	685 14-33-O

The category is defined as Higher Olefins. This category consists of discrete chemicals with an incremental change across its members. This includes:

- Olefins with even and odd carbon numbers
- Both alpha and internal olefins, referring to the position of the olefinic double bond
- Linear and branched (alkyl side chains with no other functional groups included)

Iv. EVALUATION OF EXISTING HEALTH EFFECTS DATA AND PROPOSED TESTING

A large body of data exists for aliphatic alpha and internal olefins (see Tables 6 and 7). The C6 – C 14 alpha olefins (even carbon numbers) are sponsored under the OECD SIDS High Production Volume Chemicals Program.

Based on the data that are available, the mammalian toxicity profile for the Higher Olefins is not affected by changes in the location of the double bond or the addition of branching to the structure. The only adverse health effects that have been seen are mild eye and skin irritation (in most cases not meeting regulatory criteria for irritants), lung damage/death caused by aspiration of the liquid products, and male rat nephropathy which is not considered to be relevant for human health.

Existing data show similar results in acute toxicity studies with alkenes ranging in carbon number from C6 to C24, alpha and internal, and linear and branched. Similar results were also seen in repeated-dose studies with C6, C8 and C 14 linear alpha olefins, Cl 6/C18 internal olefins (25-30% branched), and C20-24 internal olefins (approximately 40% branched).

Many of the homologs within the series, both alpha and internal, and branched and linear, have been tested for genotoxicity. All studies except two were negative. A C6 branched and linear internal alkenes blend produced a weakly positive response in a mouse micronucleus study using oral administration. However, when the study was repeated using an inhalation route, the results were negative. The Ames Test was also negative. Mouse micronucleus tests with 1-hexene and with a C6-8, C7 rich, internal branched and linear alkenes blend were negative by the oral route of administration. Another C6 alkene, neohexene, produced a slight increase in mutant frequency in the mouse lymphoma test at the highest dose level. As there was no dose response and the increase was slight, the biological significance of this response is questionable. Based on the weight of evidence, the compounds within the category are not genotoxic.

The identified adverse health effects of higher olefins (mild irritation, aspiration hazard) appear to be related to their physical rather than to their chemical properties. As the length of the olefin carbon chain increases, the materials become waxy/solid rather than liquid. The point at which the change from liquid to solid occurs appears to be affected by the change in location of the double bond and/or the degree of branching. For example, the C20-24 internal

branched and linear material is a liquid at room temperature while the linear alpha product is a solid. The predicted adverse human health effects (irritation and aspiration) of these materials is highest at the low end of the carbon range, and is expected to decrease as the carbon number and viscosity increase. Male rat nephropathy was reported on subchronic administration of C6 and Cl 4 linear alpha olefins, but was not seen in the C 16/C 18 or in the C20-24 internal branched and linear alkenes, and is not considered to be relevant for human hazard assessment.

To test the hypothesis, at the lower molecular weight end of the series, that internalizing the location of the double bond and/or changing the structure from linear to branched does not change the toxicity profile, the HPV battery of tests with an internal olefin at the low end of the category (C6 internal olefin stream containing approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes, 60-74% branched) will be completed for all mammalian toxicity endpoints and the results compared with available data for 1-hexene. To complete the HPV battery, an OECD 422, 28-Day Repeated Dose Rat Oral/Neuro/Reproduction/Developmental Toxicity Screen will be conducted. Adequate data exist for the other endpoints.

We will also test this same hypothesis near the upper molecular weight end of the series by conducting an OECD 42 1 Rat Oral Reproduction/Developmental Toxicity Screen with a C 18 mostly linear (20-30% branched) internal olefin. These results will be compared with similar data from an OECD 422 study on 1-tetradecene. These results will also be compared with data from an OECD 408 rat 90-day repeated-dose toxicity study with a C20-24 branched and linear (approximately 40% branched) internal olefins fraction. The OECD 421 test will also serve to confirm a lack of reproductive or developmental toxicity in the members near the upper end of the series. The Cl 8 internal olefin that will be tested is not an HPV material and is not a member of the category; however, it is a component of one of the members of the category and represents the upper end of the series of internal olefins within the category.

Since the upper end of the alpha olefin series of olefins is a waxy solid that is not likely to be bioavailable, and repeated dose toxicity and reproductive/developmental toxicity data exist for the more bioavailable Cl4 alpha olefin, testing of the C24 – C54 alpha olefin was not considered useful in characterizing the hazard potential of the category or appropriate, taking animal welfare considerations into account.

Summary:

<u>Acute Toxicity:</u> Acute toxicity studies exist for materials at both ends of the carbon number ranges in the series of olefins within this category and for many of the homologs within the series. The results are consistent throughout the category. Consequently, no acute toxicity testing is planned for this category.

<u>Repeated Dose and Reproductive/Developmental Toxicity</u>: Repeated dose toxicity and reproduction/developmental studies exist for C6 and Cl4 alpha olefms. Repeated dose toxicity studies exist for C16/C18 (25-30% branched) and C20-24 (approximately 40%

branched) blends of internal olefms. Results from alpha and internal olefins, whether linear or branched, or low or high carbon numbered, are consistent. A 28-day repeated dose oral/neuro/reproduction/developmental toxicity study in rats (OECD 422) will be conducted with a C6 internal olefm stream (containing approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes, 60-74% branched). An oral reproduction/ developmental toxicity screen in rats (OECD 421) will be conducted with a Cl8 mostly linear (20-30% branched) internal olefin. The results from these tests will be compared with the existing data. If the results are consistent, these data will be considered adequate to address the potential health hazards of the category.

Genetic Toxicity: Tests for gene mutation and chromosome aberrations exist for C6 and C18 linear alpha olefins and for a C6 internal olefin stream (containing approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes, 60-74% branched) and for a C20-24 internal olefins (40% branched), and for several of the homologs within those ranges. Based on the weight of evidence, these compounds are not genotoxic . No genetic toxicity testing is planned for this category.

V. EVALUATION OF EXISTING PHYSICOCHEMICAL AND ENVIRONMENTAL FATE DATA AND PROPOSALS FOR ADDRESSING THESE ENDPOINTS

Phvsicochemical Properties

Physicochemical data for each of the members of the Higher Olefins category will be developed using the EPIWIN© model (Ref. 1), as discussed in the EPA document titled "The Use of Structure-Activity Relationshins (SAR) in the High Production Volume Chemicals Challenge Program." In addition, measured physicochemical data will be provided for selected product streams in this category where readily available.

Biodegradation

Existing data show that selected chemicals in this category can biodegrade aerobically to a large extent within a few weeks and, for some chemicals, the data show that they fit the OECD criteria for Ready Biodegradability. The C6 – C 16 alpha olefins have been shown to degrade to an extent of approximately 21 to 77% in standard 28-day biodegradation tests. Results of studies for two higher molecular weight olefins (a Cl8 linear alpha olefin and a C20-24 branched and linear internal olefin) suggest that the higher alpha olefins have the potential to exhibit a significantly high, >60%, extent of biodegradation. Theoretically, the branched olefins might be expected to be significantly less biodegradable. However, the existing data do not support this supposition. Testing in an OECD 301B test with a C20-24 branched and linear material (approximately 40% branched) resulted in 92% degradation in 28 days. Sufficient data are available to assess the potential biodegradability of this category. Therefore, no additional biodegradation tests will be conducted.

Photodegradation, Hydrolysis, and Fugacity

The endpoints for photodegradation, hydrolysis, and fugacity will be either calculated or discussed. Chemical equilibrium models are used to calculate fugacity, which is only calculated. The lower homologs in the Higher Olefins category (C6 – C14) are calculated to partition primarily to the air, and therefore their fate in air is of environmental relevance (this aspect is discussed below under photodegradation). In addition, these components have relatively low Kow values, which suggests that they will not tend to partition to suspended organic matter in air and precipitate to aquatic and terrestrial compartments. The higher homologs in the category are calculated to partition primarily to the soil and sediment.

1. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (Ref. 2). UV light absorption of the substances in the category will be evaluated to identify those having the potential to degrade in solution. For those compounds with a potential for direct photolysis in water, first order reaction rates will be calculated.

2. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured (Ref. 3) (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA (Ref. 4). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation is a result of hydroxyl radical attack and is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model. Hydrocarbons, such as the majority of the chemicals in the Higher Olefins category, readily volatilize to air. In air, chemicals may undergo reaction with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (Ref.1) is used by OPPTS (the EPA's Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall hydroxyl radical (OH) reaction rate constant, a 12-hr day, and a given OH concentration. This calculation will be performed for the substances in the category.

3. Stability in Water (Hydrolysis Testing and Modeling)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Ref. 5). Stability in water can be measured (Ref. 3) (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (Ref. 4). An estimation method accepted by the EPA

includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows) (Ref. 1) is used by OPPTS.
All of the chemical structures included in the Higher Olefins category are simple hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate. A technical document will be prepared describing the potential hydrolysis rates of these substances, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

4. Chemical Distribution In The Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distibution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Ref. 6). EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (Ref. 3), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for substances in this category. A computer model, EPIWIN – version 3.02 (Ref. 1), will be used to calculate the properties needed to run the Level I EQC model.

Summary:

Phvsicochemical Properties: Physicochemical data will be calculated for representative chemicals in this category. In addition, measured physicochemical data will be provided for selected product streams in this category where readily available.

Biodegradation: Adequate data exist to characterize the aerobic biodegradation potential of the category. No biodegradation testing is planned for this category.

Photodegradation and Hydrolysis: AOP data will be calculated for representative chemicals in this category. In addition, the potential for chemicals in this category to undergo direct photolysis in water will be assessed. A technical discussion on the potential of substances in this category to hydrolyze will be prepared.

Fugacity: data will be calculated for representative chemicals in this category.

VI. EVALUATION OF EXISTING ECOTOXICITY DATA AND PROPOSED TESTING

Aquatic endpoints for the HPV Chemical Program include acute toxicity to a freshwater fish and invertebrate, and toxicity to an alga. The product streams of this category are expected to cause a narrow range of toxicity to these species within the range of solubilities acceptable for measuring acute toxicity, which for this category includes those C6 through approximately Cl0 olefins. This initial assessment is based on existing data for products that can be used to read across to this category and results of computer modeling using ECOSAR for selected chemical components of product streams in this category [ECOSAR is an aquatic toxicity modeling program and is a subroutine contained in EPIWIN']. The relatively narrow range of toxicity for the lower molecular weight members of the category is not unexpected because:

- Constituent chemicals of product streams in this category are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis and whose potencies are equivalent within the range of solubilities acceptable for measuring acute toxicity, which for this category includes those C6 through approximately C 10 olefins.
- Although the bond location is different for alpha olefins and internal olefins, the aquatic toxicities are anticipated to be similar.

The toxic mechanism of short-term toxicity for these types of chemicals is disruption of biological membrane function, and the differences between measured toxicities (i.e., LC/LL50, EC/EL50) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals. The existing fish toxicity database for narcotic chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between 4-5 mmol/kg fish (wet weight), and supports the assessment that these chemicals have equal potencies within the range of solubility that results in toxicity. When normalized to lipid content, the CBR is approximately 50 umol of hydrocarbon/g of lipid for most organisms.

The higher olefins addressed in this HPV program are essentially alpha olefins, internal olefins, and mixtures of olefins with varying degrees of branching and carbon chain length. The nature of these materials suggests that: 1) toxicity does not differ with bond location, alpha compared to internal, and 2) branching is not a major factor in toxicity for this class of chemicals. The examples shown in the tables below, illustrate this point. EPIWIN was used to estimate product solubility and octanol/water partitioning. The log Kow was used in the EPA ECOSAR toxicity estimation program.

In Table 2, the acute toxicities of fish, *Daphnia* and algae are compared from the ECOSAR estimates. A clear series of increasing acute toxicity with increase in carbon length is

observed. Also, the water solubility decreased greatly with increasing carbon chain length. Another set of ECOSAR model predictions for both alpha and internal olefins in Table 3 shows similar toxicity regardless of the nature of the bond location.

Table 2. MIXED INTERNAL OLEFINS ▪ ACUTE TOXICITY ESTIMATED FROM ECOSAR

Chemical	CAS #	fish 96h LC50 (mg/L)	Daphnid 48h LC50 (mg/L)	greenalgae 96hEC50 (mg/L)	water solubility (calculated) (mg/L)	log Kow (KowWin estimated)
hexene	25264-93-l	6.16	7.10	4.72	30.32	3.07
heptene	25339-56-4	0.83	1.03	0.73	3.35	4.13
octene	25377-83-7	0.83	1.03	0.73	3.35	4.13
nonene	27215-95-8	0.38	0.48	0.35	1.41	4.55
dodecene	25378-22-7	0.017	0.025	0.020	0.049	6.10
hexadecene	26952-14-7	no CAS # match in ECOSAR				
octadecene	27070-58-2	4.51E-05	7.87E-05	7.38E-05	7.40E-05	9.04

A comparison of predictions for l-, 2-, and 3- hexene for fish, *Daphnia* and algae show similar toxicity within each individual species. This is in part resulting from the partitioning coefficient predictions discussed earlier in the section. The prediction is consistent through 1- and 5- decene with toxicity increasing with carbon chain length and no difference between bond location either internal or in the alpha position. A third point made to confirm toxicity related specifically to partitioning coefficient for narcosis chemicals is shown in Table 4 where the degree of branching is compared for toxicity within a specific olefin and across the series. There is little or no difference in toxicity of the listed olefins when equal carbon number is compared. The three groups shown in Table 4 are predicted to have similar aquatic acute toxicity if carbon numbers are equal. The degree of branching does not have a specific effect.

Product solubility in solution during toxicity testing is critical to understanding both observations and estimates of effects. For acute toxicity, the existing data (Table 5) indicate that through the C 10 olefins, acute toxicity can be observed. Solubility is within the range of observed acute toxicity. For an internal decene stream, the acute toxicity to fish was observed to be 0.12 mg/L and the corresponding estimated solubility using ECOSAR suite is

2.51 mg/L. The effects seen in algae, Daphnia, and fish are approximately equal at water solubility. However, since that value is the LC50, there were concentrations above the LC50 of 0.12 mg/L that may not have been in solution. Above Cl0 the olefins are insoluble at levels that could cause acute toxicity and data become not usable. The results for tetradecene and higher carbon numbers indicating LC50 > 1000 mg/L only show that there was no toxicity at any exposure concentration. The solubility was too low to have resulted in toxicity. Therefore, meaningful acute toxicity data can be identified below Cl0 where solubility is high enough to allow the acute effects to be expressed.

(Table 3. ALPHA & INTERNAL OLEFINS - ACUTE TOXICITY ESTIMATED/ FROM ECOSAR

Chemical	CAS #	fish 96h LC50 (mg/L)	daphnid 48h LC50 (mg/L)	green algae 96h EC50 (mg/L)	water solubility (calculated) (mg/L)	Log Kow (KowWin estimated)
1-hexene	592-41-6	5.18	6.01	4.01	25.13	3.15
t-2-hexene	4050-45-7	6.16	7.10	4.72	30.32	3.07
t-3-hexene	13269-52-8	6.16	7.10	4.72	30.32	3.07
1-heptene	592-76-7	2.09	2.51	1.73	9.27	3.64
t-2-heptene	14686-13-6	2.49	2.97	2.03	11.19	3.56
t-3-heptene	14686-14-7	2.49	2.97	2.03	11.19	3.56
1-octene	111-66-0	0.83	1.03	0.73	3.35	4.13
t-2-octene	13389-42-9	0.96	1.19	0.84	3.95	4.06
3-octene (E)	14919-01-8	0.96	1.19	0.84	3.95	4.06
t-4-octene	14850-23-8	0.96	1.19	0.84	3.95	4.06
1-decene	872-05-9	0.12	0.16	0.12	1.04	5.12
t-5-decene	7433-56-9	0.14	0.19	0.14	1.21	5.04
1-dodecene	112-41-4	0.017	0.025	0.020	0.049	6.1
1-octadecene	112-88-9	4.51E-05	7.87E-05	7.38E-05	7.40E-05	9.04

Determining the aquatic toxicity of products that have relatively low water solubility and higher vapor pressure, like those in this category, can be difficult because they tend not to remain in solution. These data show that the measured and calculated values are in good agreement through octene, and they also support that the test methods used procedures that were able to maintain exposures.

The testing will include an alga toxicity test (OECD Guideline 201) and a *Daphnia* sp. acute toxicity test (OECD Guideline 202) on a C6 branched (60-74%) internal olefin to fill the data gaps at the lower end of the homologous series of internal olefins. This material is representative of the low end of the higher olefin category based upon the estimates in Tables *2, 3,* and 4.

Table 4. BRANCHED OLEFINS - ACUTE TOXICITY ESTIMATED FROM ECOSAR

Chemical	CAS #	fish 96h LC50 (mg/L)	daphnid 48h LC50 (mg/L)	green algae 96h EC50 (mg/L)	water solubility (calculated) (mg/L)	log Kow (KowWin estimated)
2-methyl-1-pentene	763-29-1	4.55	5.30	3.55	21.82	3.21
4-methyl-1-pentene	691-37-2	6.02	6.96	4.63	29.62	3.08
3,3,-dimethyl-1-butene	558-37-2	6.57	7.56	5.02	32.53	3.04
2-methyl-1-hexene	00604-02-6	1.84	2.21	1.53	8.06	3.70
2-methyl-1-heptene	15870-10-7	0.73	0.91	0.64	2.91	4.19
2,4,4,-trimethyl-1-pentene	107-39-1	0.92	1.14	0.80	3.77	4.08

Summary:

The lower homologs of the Higher Olefins category are sufficiently water soluble to produce acute aquatic toxicity, as has been reported for C6 – Cl0 alpha and internal olefms. The higher molecular weight olefms, those greater than C12, whose water solubilities are low, are not expected to cause acute aquatic toxicity based on the available data for selected substances. Testing with water accommodated fractions of C14, C16, and C20-24 alpha olefins and C16, C18, and C20-24 internal branched and linear olefms showed no aquatic toxicity in acute tests with fish, invertebrates, and algae. The available data, as shown in Table 5, indicate that water solubility (which is inversely proportional to the length of the alkyl chain), and not the position of the olefmic double bond (alpha or internal) or branching, influences whether a substance will produce acute aquatic toxicity. Acute toxicity tests with *Daphnia magna* and an alga species will be conducted with a C6 branched (60-74%) internal olefin (containing

approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes) to fill the data gaps at the lower end of the homologous series of internal olefins. The testing will include an alga toxicity test (OECD Guideline 201) and a *Daphnia* sp. acute toxicity test (OECD Guideline 202).

In addition, the aquatic toxicity of selected olefins will be modeled and the data used to further support the expected acute aquatic toxicity of this category.

VII. TEST PLAN SUMMARY

The following testing, modeling, and technical discussions will be developed for the Higher Olefins category (Table 8):

- To test the hypothesis, at the lower end of the series, that internalizing the location of the double bond and/or changing the structure from linear to branched does not change the toxicity profile, the HPV battery of tests with a branched (60-74%) internal olefin at the low end of the category (C6 internal olefin stream containing approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes) will be completed for all mammalian toxicity endpoints and the results compared with available data for 1 -hexene. An OECD 422, 28-Day Repeated Dose Rat Oral/Neuro/Reproduction/Developmental Toxicity Screen, will be conducted. Adequate data exist for the other endpoints.

- The location of the double bond and/or changing the structure from linear to branched is not expected to affect the level of aquatic toxicity to a significant degree based on results of modeling (ECOSAR, Ref. 1) for selected lower molecular weight alpha and internal olefins (C6 - 10). To adequately characterize the aquatic toxicity endpoints for the lower molecular weight olefins, two aquatic toxicity studies, the Algal (OECD 201) and Acute Daphnid Toxicity (OECD 202) Tests, will be conducted with a C6 branched (60-74%) internal olefin stream containing approximately 76% C6 alkenes, 16% C6 alkanes, 7% C7 alkenes. In addition, modeling for other selected lower molecular weight olefins will be conducted to support existing data and to fully characterize the algal and acute fish and invertebrate toxicity range of olefins.

- To test the hypothesis, near the upper end of the series, that changing the location of the double bond or changing the structure from linear to branched does not change the toxicity profile, an OECD 421 Rat Oral Reproduction/Developmental Toxicity Screen will be conducted with a C 18 branched and linear internal olefin (20-30% branched) and the results will be compared with data for 1-tetradecene, for which there is available an OECD 422 study, and for C20-24 branched and linear internal olefins, for which there is available an OECD 408 rat 90-day repeated-dose toxicity study. This test will also serve to confirm a lack of reproductive or developmental toxicity in the members near the upper end of the series.

- A technical discussion on the potential of representative chemicals in this category to

photodegrade will be prepared and atmospheric oxidation potentials for representative chemicals in this category will be calculated.

- A technical discussion on the potential of chemicals in this category to hydrolyze will be prepared.

- Fugacity data for representative chemicals in this category will be calculated.

- Physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* will be calculated for representative chemicals in this category. In addition, measured physicochemical data will be provided for selected product streams in this category where readily available.

If the results from the above testing confirm that the toxicity profiles of all members of the Higher Olefins category are essentially the same, and/or a pattern from lower to higher carbon numbers exists, then any remaining data gaps can be considered to fall within the ranges defined by the data and no further testing will be warranted. If the results do not confirm that hypothesis, a reassessment of the category will be conducted.

Summaries of results will be developed once the data and analyses are available. This test plan is expected to provide adequate data to characterize the human health effects and environmental fate and effects endpoints for the category under the Program.

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Table 5: Algae Toxicity and Invertebrate and Fish Acute Toxicity of C6-24 Alkenes

Species	Duration	Endpoints (mg/L)	Comments
C6			
Algae			
Selenastrum capricomutum	96-hr EC50	22	1-hexene >96%. Endpoint was biomass; no attempt to prevent evaporation
Invertebrate			
Daphnia magna	48-hr EC50	30-60	1-hexene >96%.
Daphnia magna	48-hr EC50	230	I-hexene >96%. Static, test result is above water solubility; no attempt to prevent evaporation
Vertebrates			
Rainbow trout (Salmo *gairdneri)*	48-96-hr LC50	9.7, 5.6, 5.6 and 24	I-hexene >96%. Semi-static, minimal headspace to prevent losses through evaporation
Rainbow trout *(Salmo gairdneri)*	96-hr LC50 96-hr LL50	6.6 12.8	Alkenes, C6 (internal branched stream). Mortality, semi-static; no headspace; WAF[1]
Zebra fish *(Brachiodanio* rerio)	96-hr LC50	25-50	1-hexene >96%. Semi-static, stirred 4 h before adding fish, glass beaker covered with a watch glass; also tested in glass-stoppered flask
C8			
Algae			
Selenastrum capricornutum	48-hr EC50	200	C6-8 AO[2] blend (C6 =48%, C7=36%, C8= 16%). Endpoint was biomass; no attempt to prevent evaporation; reported value exceeds water solubility limit
Invertebrate			
Daphnia magna	24-hr EC50	>3.2<10	1-octene >99%. Static, stirred 4 h before adding test animals, glass beaker covered with a watch glass; also tested in glass-stoppered flask
Vertebrates			
Zebra fish *(Brachiodanio rerio)*	24-96-hr LC50	3.2	1-octene >99%. Static, stirred 4 h before adding fish, glass-stoppered flask, open and closed, nominal with t-butanol as carrier. Without t-butanol as a carrier, the 48-96 hr LC50= 4.8
Rainbow trout (Salmo *gairdneri)*	96-hr LC50 96-hr LL50	0.87 8.9	Alkenes, C7-9, C8 rich (internal branched stream). Mortality, semi-static; no headspace;WAF
Cl0 and Cl2			
Algae			
Selenastrum capricornutum	96-hr EC50	22	C10-13 AO blend (C10-11=30%, C11-12=31%, C12=11%, C13=21%). Static, vessels not sealed, solution aerated. Concentrations utilized in testing were greater than the water solubility
Scenedesmus subspicatus	72-hr E_bC50	15.4	Idodecene >97%. Endpoint was biomass: reported value exceeds water solubility limit
Invertebrates			
Daphnia magna	24-hr EC50 48-hr EC50	720 480	C10-13 AO blend (C10-11=30%, C11-12=31%, C12=11%, C13=21%). Static, vessels not sealed, solution aerated, concentrations utilized in testing were greater than the water solubility
Vertebrates			
Rainbow trout (Salmo *gairdneri)*	96-hr LC50 =	>1000	C10-13 AO blend (C10-11=30%, C11-12=31%, C12=11%, C13=21%). Semi-static, vessels not sealed, solution aerated; concentrations utilized in testing were greater than the water solubility
Rainbow trout (Salmo *gairdneri)*	96-hr LC50 96-hr LL50	0.12 4.8	Alkenes, C9-11, C10 rich (internal branched stream). Mortality, semi-static; no headspace; WAF
Rainbow trout *(Salmo gairdneri)*	96-hr LLO	86.0	Alkenes, Cl I-13, C 12 rich (internal branched stream). Mortality, semi-static; no headspace;WAF
C14			
Algae			
Selenastrum capricornutum	72- 96 hr ELO	1000	I-tetradecene 99%. Growth; static test; WAF
Invertebrates			
Daphnia magna	24-hr ELO and 48-hr ELO	1000	1-tetradecene 99%. Immobility; semi-static test
Vertebrates			
Rainbow trout (Salmo *gairdneri)*	96-hr LLO	1000	1-tetradecene 99%. Mortality; semi-static test

[1] WAF= Water Accommodated Fractions test procedure was used due to the low water solubility of the test material.

[2] AO = Alpha Olefin

Species	Duration	Endpoints (mg/L)	Comments
C16 and C18			
Algae			
Selenastrum capricornutum	72-hr ELO	1000	I-hexadecene. Growth; static test; WAF
Selenastrum capricornutum	96-hr EC50	>1000	I -octadecene. Growth; static test; concentrations utilized in testing greater than solubility; no toxicity seen at 1000 mg/l
Invertebrates			
Daphnia magna	24-hr EC50 and 48-hr EC50	>1000	1 -octadecene. Immobility; static test; concentrations utilized in testing greater than solubility
Vertebrates			
Rainbow trout (*Salmo gairdneri)*	96-hr EC50	>1000	I -octadecene. Mortality; semi-static test; concentrations utilized in testing greater than solubility; no toxicity seen at 1000 mg/l
Turbot (*Scophthalmus maximus*)	96-hr LC50	> 10,000	C16/C18 internal linear and branched blend (50/50). Mortality; semi-static test
C20-24			
Algae			
Selenastrum capricornutum	72-hr ELO	1000	C20-24 linear AO blend. Growth; static test; WAF
Selenastrum capricornutum	72-hr ELO	1000	C20-24 internal linear and branched blend. Growth; static test; WAF
Invertebrates			
Daphnia magna	48-hr ELO	1000	C20-24 internal linear and branched blend. Immobility; static test
Vertebrates			
Rainbow trout (*Oncorhynchus mykiss)*	96-hr LLO	1000	C20-24 linear AO blend. Mortality; semi-static test; WAF
Rainbow trout (*Oncorhynchus mykiss)*	96-hr LLO	1000	C20-24 internal linear and branched blend. Mortality; semi-static test; WAF

Table 6. Existing Data for Higher Olefins

Alpha Olefins															
		Human Health Effects						Ecotoxicity			Environmental Fate				
Chemical Name	CAS #	Acute Toxicity	Genetic Point Mutation	Genetic Chrom. Aberr.	Sub-chronic	Developmental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photodegradation	Hydrolysis	Fugacity	Biodegradation
1-Hexene[1]	592-41-6 Linear	√	√	√	√	√	√	√	√					√	√
Neohexene	558-37-2 Branched	√	√												
1-Octene[1]	111-66-0 Linear	√	√	√	√			√	√					√	
1-Decene[1]	872-05-9 Linear	√	√												√
1-Dodecene[1]	112-41-4 Linear	√	√	√	√			I	I	√[5]					
1-Tetradecene[1]	1120-36-1 Linear	√	√	√	√	√	√	√	√	√				√	√
1-Hexadecene[2]	629-73-2 Linear	√	√	√				√		√					√
1-Octadecene[2]	112-88-9 Linear	√[3]	√	√				√[6]	√[6]	√[6]					√
C12-16[4] (even numbers)	see C12,14, 16 above Linear		√	√											
C14-18 (even numbers)	68855-59-4 Linear	√													
C20-24 (even numbers)*	93924-10-8 Linear	√						√		√					
C22-28 (even numbers)*	93924-11-9 Branched and Linear	√													
C24-54 (even numbers)*	131459-42-2 Branched and Linear	√													

√ Adequate existing data available

I Robust Summaries will not be submitted, summaries are available in the OECD SIDS dossiers.

2 Robust Summaries will be submitted separately.

3 Cl 8-C24 and C18-C26 blends (even cation numbers) were tested.

4 Robust Summaries will not be submitted; summaries are available in the OECD SIDS dossier for 1-tetradecene.

5 Result questionable because EC50 value is above the water solubility.

6 Some concentrations tested were above water solubility and too few concentrations used to consider high quality data.

Table 6. Existing Data for Higher Olefins (Continued)

(Robust summaries for these studies will be submitted separately)

Internal Oletins																
		Human Health Effects						Ecotoxicity			Environmental Fate				
Chemical Name	CAS #	Acute Toxicity	Genetic Point Mutation	Genetic Chrom. Aberr.	Sub-chronic	Develop-mental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem	Photo-degradation	Hydro-lysis	Fugacity	Biodegradation
Alkenes, C6	68526-52-3 (60-74% branched)		√	√				√							√
C7-rich Alkenes, C6-8,	(60-74% branched)	√		√											
Alkenes, C7-9, C8-rich	68526-54-5 (60-74% branched)	√						√							√
Alkenes, C8-10, C9-rich	68526-55-6 (60-74% branched)	√	√	√											
Alkenes, C9-11, C10 rich	68526-56-7 (60-74% branched)							√							√
Alkenes Cl 1-13, C 12-rich	68526-58-9 (60-74% branched)	√						√							√
Alkenes, C12-14, Cl3 Rich	68526-58-9 (60-74% branched)														√
C16/C18	Various (20-30% branched)	√[1]			√[2]			√[3]							√[3]
C20-24	various (appmx. 40% branched)	√	√	√	√			√	√	√					√
C24-30	Various (appmx. 40% branched)	√	√												√

√ Adequate existing data available

1 C16 and Cl8 tested separately.

2 54% C16, 38% C18, 8% C20, 2% linear alpha, 72% linear internal, 26% branched.

3 50% C16 and 50% C18

Table 7: Health Effects of C6-54 Alkenes

	Acute Toxicity	Repeated Dose	Mutagenicity In Vitro	Mutagenicity In Vivo	Repro/Dev
C 6	Oral: Rat LD50>5600 mg/kg and >10,000 mg/kg [1-hexene]; >5000 mg/kg [neohexene] Inhalation: Rat LC50 (4hr) = 32,000 ppm (nom) [1 -hexene]; >5 1,000 ppm [neohexene]	1 -hexene Rat, 90day inhalation OECD 4 13; NOEL= 1000 ppm Rat, 28day gavage OECD 407; NOEL= 10 1 mg/kg (gastric effects [males and females] and reduced body weights [males only]) Rat oral OECD 421; NOEL <100 mg/kg (general tox -male rat nephropathy)	1-hexene: *S. typhimurium*, OECD 47 1 w/out repeat assay; Mouse Lymphoma, OECD 476, Mammalian Ceil gene mutation ; CHO and Human lymphocytes-Metaphase Chromosome Analysis, OECD 473. All negative with and w/out activation UDS-rat hepatocyte; OECD 482; Negative at 0.5 and 2 mg/ml; no evaluation at 3.5 and 5.0 mg/mL due to toxicity. BALB/3T3 cells transformation: Negative neohexene: *S. typhimurium*, OECD 47 1 w/out repeat assay and CHO SCE, OECD 479, negative with and w/out activation; Mouse Lymphoma Mammalian Cell gene mutation, OECD 476, weakly positive w/out S9 w/out dose response Alkenes, C6 (internal branched stream): *S. typhimurium*, OECD 471, negative with and w/out activation	1-hexene and alkenes, C6 (internal branched stream): Mouse Bone Marrow micronucleus, OECD 474 (inhln); negative at 0, 1000, 10000 and 25000 ppm [1-hexene] and 1000 ppm [alkenes, C6] Alkenes, C6 (internal branched stream): Mouse Bone Marrow micronucleus, OECD 474 (oral); weakly positive at 5 g/kg	1 -hexene Rat; OECD 42 I ; doses at 0, 100, 500, and 1000. NOEL=> 1000 mg/k (reproductive tox, parental, adult female); NOEL => 1 OOOmg.kg (reproductive tox, F1 generation); NOEL=> 1000 mg/k (Pregnancy litter); NOEL=> 1000 mg/k (foetal data)
c 7	Alkenes, C6-8, C7 rich (internal branched stream): Inhalation: Rat, mouse and guinea pig LC50 (6hr) >42.3 mg/L Dermal: Rabbit LDSO >3 160 mg/kg (24 hr)			Alkenes, C6-8, C7 rich (internal branched stream): Mouse Bone Marrow micronucleus, OECD 474 (oral); negative	
C8	Oral: Rat LD50> 10g/kg and >5 ml/kg [1 -octene]; >5g/kg [alkenes., C7-9, C8 rich internal branched stream] Inhalation: Rat LC50 (4 hr) = 8,050 ppm (nom) [1 -octene]; rat and mouse LC50 (6	1 -octene Rat, 90 day oral (gavage) dosing at 0,5,50 or 500 mg/kg/bw - NOEL = 50 mg/kg/day increased kidney weights and decreased plasma chloride in both sexes	-octene: *Styphimurium* and BALB/c-3T3 transformation: Negative with and w/out activation Two CHO chromosome abberrations		

	hr) > 3 1.7 mg/L and guinea pig LC50 (6 hr) < 3 1.7 mg/L [alkenes, C7-9, C8 rich internal branched stream] Dermal: Rabbit LD50 >10 g/kg (24 hr) and 1.43 g/kg (24 hr) [1-octene]; >3.16 g/kg (24 hr) [alkenes, C7-9, C8 rich internal branched stream]		tests; one was negative with and w/out activation and the other had questionable results with activation; (aberration rate increased approx 2-fold over background, but no dose response) and was negative w/out activation.		
c 9	Alkenes, C8-10, C9 rich (internal branched stream): Oral: Rat LD50>2332 m&g Inhalation: rat LC50 (6 hr) > 1 1.1 mg/L Dermal: Rabbit LD50 >2332 m&g (24 hr)		Alkenes, C8-10, C9 rich (internal branched stream): *S.typhimurium* OECD 47 1: Negative with and w/out activation	Alkenes, C8-10, C9 rich (internal branched stream): Mouse Bone Marrow micronucleus, OECD 474 (oral); negative at doses of 1.25, 2.5 and 5 g/kg	
C10	1 -decene Oral: Rat LD50> 10g/kg Inhalation: Rat LC50 >saturation conc for 1 and 4 hr exposure at saturation of 9.3 and 8.7 mg/L Dermal: Rabbit LD50 > 10 g/kg (24 hr)		1 -decene. *S.typhimurium*; OECD 47 1; Negative with and w/out activation		
C12	Oral: Rat LD50>7.7 g/kg, >10 g/kg and > 1 0g/kg [I dodecene]; >7.74 g/kg [alkenes, Cl I-13, Cl2 rich internal branched stream] Inhalation: Rat LC50 (4 hr) > 2. I mg/l [CIO-13 AO]; (lhr) >9.9 mg/L [C12, 14, 16 linear AO blend]; rat, mouse and guinea pig LC50 (6 hr) > 4.4 mg/L [alkenes, Cl 1-13, Cl2 rich internal branched stream] Dermal: Rat LD50 > 3.04 g/kg [C10-13 AO blend] and >10 g/kg [1 dodecene]; rabbit LD50 >2446 mg/kg (24 hr) [alkenes, Cl I-13, Cl2 rich internal branched stream]	C12, 14, 16 linear AO blend: Dermal: Rabbit; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg; severe irritation and decrease in bodyweight seen with 2 g/kg; slight irritation seen with 1 g/kg;	*S. typhimurium* and *E.coli* [blend of Cl 1-12 AO[3]; Idodecene]; CHO/HGPRT [blend of C12, Cl4 and C 16 linear AO]; *S. cerevisiae* Mitotic Gene conversion Assay [Cl 1-12 AO blend and Idodecene]: All negative with and w/out activation CA Rat liver RL1 cells [Idodecene], CA Rat liver RL4 cells [Cl 1-12 AO blend]; BALB/c-3T3 Mouse embryo and UDS [C12, 14, 16 linear AO blend]: All negative	C 12, 14, 16 linear AO blend: Mouse Micronucleus Bone Marrow Test (dermal); No remarkable clinical findings-negative at doses of 1000.2500 and 5000 mg/kg for 2 days	
C14	Oral: Rat LD50 17.3 g/kg [C10-14 AO] and >10g/kg [C12-14, C14-18, C14-16 AO]; Mouse LD50= 21.3 g/kg [CIO-14 AO] Inhalation: Rat LC50 (1 hr) = 9900 mg/m^3 [C 1 2, 14, 16 linear AO blend]; Mouse LC50 = 223 mg/L [C10-14 AO blend] Dermal: Rat LD50 >10 g/kg [C12, 14, 16	1-tetradecene: Combined OECD 422; rat; gavage dosed at 0, 100,500 or 1000 mg/kg/bw/day for up to 5 1 days. NOAEL = 100 mg/kg/day liver effects in non-pregnant female satellite group and no NOEL for males due to kidney effects C12, 14, 16 linear AO blend: Dermal: Rabbit; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg; severe irritation	C13-14 AO blend: *S. typhimurium*, S. *cervisiae* Mitotic recombination with and w/out activation; CA Rat Liver RLI cells: Negative C12, 14, 16 linear AO blend: UDS (rat hepatocyte), CHO HGPRT and BALB/c-3T3: Negative	*C12, 14, 16 linear AO blend:* Mouse Micronucleus Assay (dermal); Negative at doses of 1000, 2500 and 5000 mg/kg for 2 days.	1-tetradecene: Rat; Modified OECD 422; gavage at 0. 100,500 or 1000 mg/kg/bw/day for up to 5 I days; NOAEL parental: 1000 mg/kg/bw/day; NOAEL F1 Offspring; 1000

	linear AO blend; C12-14 AO blend; C14-18 AO blend, and C14-16 AO blend]	and decrease in bodyweight seen with 2 g/kg; slight irritation seen with 1 g/kg;			mg/kg/day No developmental effects seen through day 4 of lactation
C16	Oral: Rat LD50 >10g/kg [1-hexadecene] and >5050 mg/kg [Cl6 internal linear and branched] Inhalation: Rat LC50 = 6.4 mg/l (4hr) and >8.5 mg/l (1 hr) [I-hexadecene] Dermal: Rabbit LD50 >2020 mg/kg (24 hr) [Cl 6 internal linear and branched]	C 16- 18 internal linear and branched: Oral: OECD 407; rat; dosed at 0, 25, 150 or 1000 mg/kg/bw/day for up to 4 wks. NOAEL = 1000 mg/kg/day C12, 14, 16 linear AO blend: Dermal: Rabbit; 9 applications (6 hr) over 2 wk period of 1 or 2 g/kg; severe irritation and decrease in bodyweight seen with 2 g/kg; slight irritation seen with 1 g/kg	1-hexadecene: *S. typhimurium*: Negative with and w/out activation C12, 14, 16 linear AO blend: UDS (rat hcpatocyte) and BALB/c-3T3: Negative	1-hexadecene: Mouse Micronucleus Assay (oral); Negative at 7.85 g/kg (only dose administered). C12, 14, 16 linear AO blend: Mouse Micronucleus Assay (dermal); Negative at doses of 1000, 2500 and 5000 mg/kg for 2 days.	
C18	Oral: Rat LD50 >10g/kg [C14-18 AO blend, C IS-26 AO blend, C 18-24 AO blend] and >5050 mg/kg [C18 internal linear and branched] Dermal: Rabbit LD50 >10 g/kg (24 hr) [C1 8-24 AO blend, C 18-26 AO blend] and >2020 mg/kg (24 hr) [C 18 internal linear and branched]	C16-18 internal linear and branched: Oral: OECD 407; rat; dosed at 0.25, 150 or 1000 mg/kg/bw/day for up to 4 wks. NOAEL = 1000 mg/kg/day	1-octadecene: *S. cervisiae* Mitotic gene conversion and *S. typhimurium* with and w/out activation; CA Rat Liver RL1 cells: Negative		
C20-24	Oral: Rat LD50 >5 g/kg [C20-24 linear AO, C20-24 internal linear and branched, and C22-28 linear AO] and >15 g/kg [C20-24 linear AO] Dermal: rat LD50 >5 ml/kg (24 hr) [C20-24 linear AO] and >2 g/kg [C20-24 internal linear and branched]	C20-24 internal linear and branched: Combined OECD 408; rat gavage dosed at 0, 100,500 or 1000 mg/kg/bw/day for 90 days. NOAEL = 1000 mg/kg/day	C20-24 internal linear and branched: *S. typhimurium* OECD 47 1; and CA human lymphocytes: Negative with and w/out activation	C20-24 internal linear and branched: Mouse Micronucleus Assay (i.p.): Negative at doses of 500, 1000 and 2000 mg/kg	
C24-28	C24-28 internal linear and branched: Oral: Rat LD50 >5 g/kg		C24-28 internal linear and branched: *S. typhimurium* OECD 47 I: Negative with and w/out activation		
C24-54 (C30+)	C24-54(C30+) AO linear and branched: Oral: Rat LD50 >2 g/kg and >15 g/kg Dermal: rat LD50 >5 ml/kg (24 hr)				

Table 8. Assessment Plan for Higher Olefms Category Under the Program
(Robust summaries for existing studies will be submitted separately.)

Alpha Olefins															
		Human Health Effects						Ecotoxicity			Environmental Fate				
Chemical	CAS #	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
I-Hexene (SIDS)	592-41-6 Linear	√	√	√	√	√	√	√	√	√					√
Neohexene	558-37-2 Branched	√	√	√	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Tetradecene (SIDS)	1120-36-1 Linear	√	√	√	√	√	√	√	√	√				√	√
1-Tridecene	2437-56-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Hexadecene (ICCA)	629-73-2 Linear	√	√	√	RA	RA	RA	√	RA	√	SAR	TD	TD	CM	√
1-Octadecene (ICCA)	112-88-9 Linear	√	√	√	RA	RA	RA	√	√	√	SAR	TD	TD	CM	√
Alkenes, C 10-1 6 alpha (even carbon numbers)	68855-58-3 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C14-18 alpha (even carbon numbers)	68855-59-4 Linear	√	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C14-20 alpha (even carbon numbers)	68855-60-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1 -Eicosene	3452-07-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Docosene	1599-67-3 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
1-Tetracosene	10192-32-Z Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
a-olefin fraction C20-24 cut (even numbers)	93924-10-g Linear	√	RA	RA	RA	RA	RA	√	RA	√	SAR	TD	TD	CM	RA
a-olefin fraction C24-28 cut (even carbon numbers)	93924-11-9 Branched and Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
alkene, C24-54 branched and linear, alpha (even numbers)	131459-42-2 Branched and Linear	√	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA

√ Adequate existing data available
CM Computer Modeling proposed
TD Technical discussion proposed
SAR Structure Activity Relationship
RA Read Across (see Sec. IV & VI)
T Proposed Testing

Table 8. Assessment Plan for Higher Olefms Category Under the Program (Continued)
(Robust summaries for existing studies will be submitted separately.)

Internal Olefins															
		Human Health Effects						Ecotoxicity			Environmental Fate				
Chemical	C A S #	Acute Toxicity	Genetic Point Mut.	Genetic Chrom	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Alkenes, C6	68526-52-3 Br. and Lin.	RA	√	√	T	T	T	√	T	T	SAR	TD	TD	CM	√
Hexene (ICCA)	25264-93-1 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	C M	RA
Alkenes, C6-8, C7 rich	68526-53-4 Br. and Lin.	√	RA	√	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	R A
Heptene (ICCA)	25339-56-4 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	T D	C M	RA
Octene (ICCA)	25377-83-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	T D	C M	RA
Alkenes, C7-9, C8-rich	68526-54-S Linear or Br. and Lin.	√	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	TD	CM	√
Nonene (ICCA)	27215-95-8 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	C M	R A
Alkenes, C8-10, C9-rich	68526-55-6 Linear or Br. and Lin.	√	√	√	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C9-11, C10-rich	68526-56-7 Linear or Br. and Lin.	RA	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	T D	CM	√
C10,12 Olefinrich hydrocarbons	68514-32-9 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	R A
Alkenes, C10-12, Cl l-rich	68526-57-8 Br. and Lin.	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA

√ Adequate existing data available
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T Proposed Testing

Table 8. Assessment Plan for Higher Olefms Category Under the Program (Continued)
(Robust summaries for existing studies will be submitted separately.)

Internal Olefins (continued)																
		Human Health Effects						Ecotoxicity			Environmental Fate				
Chemical	CAS #	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Reproduc-tion	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photo-deg.	Hydro-lysis	Fugacity	Biodeg.
Alkenes, C11-13, C12-rich	68526-58-9 Linear or Branched or Br. and Lin.	√	RA	RA	RA	RA	RA	√	RA	RA	SAR	TD	TD	CM	√
Dodecene (ICCA; not sponsored in HPV)	25378-22-7 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Heavy polymerization naphtha (petroluem)	68783-10-8 Branched	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
C12,14 Olefin rich hydrocarbons	68514-33-0 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C10-16	68855-58-3 Linear	RA	RA	RA	RA	RA	RA	RA	RA	RA	SAR	TD	TD	CM	RA
Alkenes, C15-C18	93762-80-2 Linear	RA	RA	RA	RA	RA	RA	√	√	√	SAR	TD	TD	CM	RA
Octadecene (Not HPV and not sponsored under HPV ; data used to support category)	Various Branched and Linear	√			√	T	T	√	√	√					√
C20-24 (Not HPV and not sponsored under HPV; data used to support category)	Various Branched and Linear	√	√	√	√			√	√	√					√

√ Adequate existing data available
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RA **Read Across (see Sec. IV & VI)**
T **Proposed Testing**